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**Structural, Magnetic and Electrical Properties
of the New Ternary CePdIn₂**

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ABSTRACT

CePdIn₂ is found to crystallize in the orthorhombic space group *Cmcm* (*Z*=4) with *a* = 4.6210(9) Å, *b* = 10.694(2) Å, and *c* = 7.455(2) Å. Single crystal X-ray data were refined to *R* = 0.0459 (*wR*₂ = 0.0666), with 255 independent reflections and 16 variables. The structure adopts the BRe₃ structure type and is the first known Ce-containing member. Magnetic measurements indicate that CePdIn₂ undergoes a ferromagnetic phase transition with a *T*_c near 10 K. The electrical resistivity of CePdIn₂ shows metallic behavior with a small anomaly at the magnetic phase transition.

INTRODUCTION

Over the past 20 years, research in ternary cerium intermetallics has grown substantially as interesting strongly correlated electron systems have been observed (1,2,3). While much progress has been made in understanding the origin of these effects, this knowledge is insufficient to predict new compounds which exhibit these phenomena.

However, as discussed by Fisk et al. (4), the chemical composition of the interesting Ce compounds includes mostly elements in the late transition metal and early p block columns. In particular, in the Ce-Pd-In ternary phase diagram, there are a number of interesting correlated electron materials such as CePd_3 (5), CeIn_3 (6), and CePdIn (7).

Motivated by the unusual materials found in this system as well as more recently discovered compounds (8), we have been searching for other new ternaries in this phase space (9). Here, we report the structure and properties of a new compound, CePdIn_2 .

EXPERIMENTAL

Sample Preparation

CePdIn_2 was synthesized by arc-melting stoichiometric amounts of the elements on a water-cooled, Ta coated copper hearth under a flow of Ti-gettered Ar (Centorr Furnaces, Model 2B-20). The arc-melted beads were flipped over and remelted repeatedly to increase homogeneity. Mass losses after arc-melting were less than 0.5%.

The elements used were all at least of purity 99.9%. The cerium was further purified by vacuum melting into a water-cooled copper cup, leaving behind much of the outer oxide coat often present on Ce pieces.

The arc-melted beads were then placed in tantalum tubing and sealed in quartz under vacuum. The beads were then heated at 825 °C for one week.

Structure determination

Preliminary structure characterization was done with electron and x-ray diffraction of finely ground powder. Electron diffraction patterns were obtained using powder suspended on holey carbon coated grids in a double tilt holder in a JEOL 1200 EX transmission electron microscope. The powder was also studied by X-ray diffraction using a Scintag XDS 2000 diffractometer with Cu K α radiation. The diffraction data indicated an orthorhombic cell of approximate dimensions 4.621 x 10.692 x 7.450 Å and C-centering.

Shards of lightly cracked beads were mounted and screened for crystal quality using precession camera photos. Single crystal data were collected on a Siemens P4 four-circle diffractometer in the θ -2 θ mode from $-1 \leq h \leq 6$, $-1 \leq k \leq 13$, and $-1 \leq l \leq 9$. The lattice constants for the cell were $a = 4.6210(9)$ Å, $b = 10.694(2)$ Å, and $c = 7.455(2)$ Å, in good agreement with the powder data. Three check reflections were measured every 50 reflections, and they showed no evidence of crystal decomposition or movement on the fiber. An empirical psi-scan absorption correction was applied to the data, yielding an $R_{\text{int}} = 0.0305$. The semi-invariants representation program SIR92 (10) was used to generate a model for the structure which was refined with XL from the SHELXTL

version 5y program (11). The final structure R values were $wR_2 = 0.0666$ and $R_1 = 0.0459$ for all data and $wR_2 = 0.0614$ and $R_1 = 0.0310$ for $I > 2\sigma(I)$. The MISSYM algorithm (12) detected no further symmetry elements than those expected for Cmc₂m.

Crystal structure data, values of the atomic parameters, and anisotropic displacement parameters are listed in Tables 1, 2, and 3. The atomic positions are presented both in accordance with previous BRe₃ structure literature and also in the standard format as determined by the program STRUCTURE TIDY (13). This program standardizes inorganic structures to help identify similar structures, obscured by differences in the reporting of crystal data.

Additional structure information, including structure amplitudes, is available as supplementary material.¹

Physical property measurements

The magnetic susceptibility of CePdIn₂ was measured using a Faraday balance on coarsely ground, loose powder. The field dependence of the susceptibility at room temperature from 2.1 kG to 14.6 kG showed variations of less than 1%, indicating the absence of ferromagnetic impurities. Temperature dependent data from 4 to 325 K were collected in a field of 10 kG. Platinum was used as a calibration standard. The measured room temperature susceptibility of Pt $\chi(293\text{ K})$ was 1.030×10^{-6} emu/g, in good agreement with a literature value of 1.035×10^{-6} emu/g (14).

Electrical resistivity was measured using standard four probe AC techniques. The contacts were ohmic by linearity of the I-V curve. The

resistivity sample was bar-shaped, cut with a string saw from a bead after heat treatment.

RESULTS AND DISCUSSION

Structural Aspects

The structure of CePdIn_2 is isotypic with the rare earth intermetallics $(\text{Y}, \text{Gd}, \text{Tb}, \text{Dy})\text{NiIn}_2$ (15), $(\text{Y}, \text{Tb-Lu})\text{NiGa}_2$ (16), $(\text{Y}, \text{Tb-Lu})\text{PdGa}_2$ (17), and $(\text{Y}, \text{Tb-Lu})\text{NiAl}_2$ (18). Thus, the structure type was previously known only for compounds containing the smaller rare earth atoms.

As shown in Figure 1, the structure can be described as a staggered net of trigonal prisms. Each prism is composed of four In atoms and two Ce atoms centered by a Pd atom.

Selected bond distances are listed in Table 4. The bond distances indicate that the chemical environment of the atoms is more complicated than emphasized in Figure 1. Figure 2 shows the coordination polyhedra around each of the atoms as determined by the principle of maximal gap in near neighbor distances (19). All resulting distances are short enough to be considered as bonding to the central atom.

As shown in Figure 2a, the 13-coordinate environment around the Ce can be described as a distorted pentagonal prism of eight In atoms and two Pd atoms with two In atoms and one Pd atom capping three square faces of the prism. The Pd environment of nine neighbors, shown in Figure 2b, consists of a trigonal prism of four In atoms and two Ce atoms, tricapped by two In

atoms and one Ce atom. The coordination geometry of In to its 12 neighbors is irregular and is depicted in Figure 2c. It consists roughly of Ce atoms in square pyramidal coordination and In atoms in tetrahedral coordination about the central In. Three Pd atoms complete the coordination polyhedron.

The complicated polyhedra suggest that size constraints strongly limit the formation of the BRe_3 structure type. An unsuccessful attempt at making $CeNiIn_2$ underscores this probable steric limitation. The larger Pd and In atoms are perhaps necessary to stabilize the structure for the larger rare earth Ce atom. To date, the presented structure is the only known Ce or Pd-In example for this structure type.

Magnetic properties

Figure 3 shows the inverse magnetic susceptibility for $CePdIn_2$ upon heating the powder sample from 4.2 K. The data were fit to the Curie-Weiss

$$\text{law: } \chi = \chi_0 + \frac{C}{T - \theta} .$$

The fit parameters were selected by choosing a temperature range of fit, fixing θ , and then determining C and χ_0 using standard analysis techniques (20). θ was varied, and for each choice, a fractional variance σ was calculated. The final parameters were chosen to minimize σ over the largest temperature range.

These parameters were found to be $\chi_0 = 2.6 \pm 0.4 \times 10^{-7}$ emu/g, $C = 1.60 \pm 0.02 \times 10^{-3}$ emu-K/g, and a ferromagnetic $\theta = 16.5 \pm 1.5$ K for the temperature

range of 75 to 325 K with a $\sigma = 1.5 \times 10^{-3}$. At temperatures below 75 K, some deviations from the Curie-Weiss law occur, most likely due to crystal field effects. The Curie constant corresponds to a moment of $2.47 \pm 0.02 \mu_B$ which is very close to the free ion value of $2.54 \mu_B$ for Ce^{+3} . Hence, it appears that in $CePdIn_2$, the Ce is trivalent, with ferromagnetic exchange. We can estimate a transition temperature of ≈ 10 K from the inflection point of the χ vs temperature curve.

As shown in Figure 4, the field dependence of the low temperature susceptibility is consistent with a ferromagnetically ordered material. Fitting the χ vs $1/H$ curve to a straight line, we obtain a magnetization at 4.2 K of $1.6 \mu_B$ vs the expected $gJ = 2.14 \mu_B$ for completely oriented Ce^{+3} ions in a $J=5/2$ state. The deviation from the expected value may indicate that there is some canting of the spins in the ordered state or more likely that crystal field splitting reduces the ground state moment.

The existence of ferromagnetism in this system agrees well with the empirical observations of Sereni and Kappler (21). They found that ferromagnetic behavior is often present in systems with Ce-Ce nearest neighbor distances between 3.7 and 4.1 Å. In $CePdIn_2$ this distance is 4.063 Å.

Electrical properties

Resistivity data from room temperature to 4.2 K are shown in Figure 5. The magnitude of the resistivity and its monotonic decrease with temperature down to ≈ 20 K indicate metallic conduction. At roughly 10 K,

there is a kink in the resistivity, most likely due to a coupling of the carriers to the ordering Ce moments.

Note that the resistivity decreases more rapidly below 10 K than just above, indicating that spin-disorder scattering may be playing a role at higher temperatures. Below the ferromagnetic transition, this extra scattering is expected to die out as the moments order. This behavior is similar to that observed in other rare earth intermetallic compounds such as NdAuAl (22) and GdNiGe (23).

CONCLUSIONS

We have synthesized a new ternary intermetallic compound, CePdIn₂, the first known Ce containing member of the BRe₃ structure type. From the magnetic and electrical properties, we conclude that CePdIn₂ is a ferromagnet with a T_c of about 10 K. It appears that the Ce moments do not interact strongly with the conduction electrons, as we see little evidence of Kondo-like magnetic or transport behavior.

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REFERENCES

1. Z. Fisk and J.R. Schrieffer, *MRS Bulletin* **28**, 23 (1993).
2. N.B. Brandt and V.V. Moshchalkov, *Adv. Phys.* **33**, 373 (1984).
3. J.M. Lawrence and D.L. Mills, *Comments Cond. Mat. Phys.* **15**, 163 (1991).
4. Z. Fisk, J.D. Thompson, and H.R. Ott, *J. Magn. Magn. Mater.* **76&77**, 637 (1988).
5. D. Jaccard, M.J. Besnus, and J.P. Kappler, *J. Magn. Magn. Mater.* **63&64**, 572 (1987).
6. J.M. Fournier and E. Gratz in K.A. Gschneidner, Jr. L. Eyring, G. H. Lander and G.R. Choppin (eds.), *Handbook on the Physics and Chemistry of Rare Earths*, Elsevier, Netherlands, **17**, 409 (1993).
7. K. Satoh, T. Fujita, Y. Maeno, Y. Uwatoko, and H. Fujii, *J. Phys. Soc. Japan* **59**, 692 (1990).
8. B. Xue, F. Hulliger, Ch. Baerlocher, and M. Estermann, *J. Alloys Compd.* **191** L9 (1993).
9. R.A. Gordon, Y. Ijiri, C.M. Spencer, and F.J. DiSalvo, *J. Alloys Compd.* **224**, 101 (1995).
10. A. Altomere, M.C. Burla, M. Camilli, G. Cascarano, C. Giacovazzo, A. Guagliardi, G. Polidori, *J. Appl. Crystallogr.*, in preparation, (1994).
11. G.M. Sheldrick, SHELXTL version 5, Siemens Analytical X-ray Instruments, Inc., Madison, WI.

12. Y. LePage, *J. Appl. Crystallogr.* **20**, 264 (1987).
13. L.M. Gelato and E. Parthé, *J. Appl. Crystallogr.* **20**, 139 (1987).
14. D.R. Lide, ed., *Handbook of Chemistry and Physics*, CRC Press, Boca Raton, **74**, 9-53 (1993).
15. V.I. Zarembo, O.Ya. Zakharko, Ya.M. Kalychak, and O.I. Bodak, *Dop. Akad. Nauk Ukrain. RSR, Seriya B* **12**, 44 (1987).
16. V.A. Romaka, Ju.N. Grin', Ja.L. Jarmoljuk, R.V. Skolozdra, and A.A. Jartys', *Ukr. Fiz. Zh.* **28**, 227 (1983).
17. Ju.N. Grin', *Dop. Akad. Nauk Ukrain. RSR, Seriya B* **9**, 34 (1984).
18. R.M. Rykhal', O.S. Zarechnyuk, and Ya. P. Yarmolyuk, *Sov. Phys. Cryst.* **17**, 453 (1972).
19. G.O. Brunner and D. Schwarzenbach, *Z. Kristallogr.* **133**, 127 (1971).
20. P.R. Bevington, *Data Reduction and Error Analysis for the Physical Sciences*, McGraw Hill, New York, (1969).
21. J.G. Sereni and J.P. Kappler, *Physica B* **171**, 166 (1991).
22. L. Menon and S.K. Malik, *Phys. Rev. B* **51**, 5858 (1995).
23. C.S. Garde, J. Ray, and G. Chandra, *J. Alloys Compd.* **201**, L5 (1993).

TABLE 1

Crystal Data and Structure Refinement for CePdIn₂

Empirical formula	CePdIn ₂
Formula weight	476.16
Diffractometer type	Siemens P4 four-circle
Radiation	Graphite monochromated MoK α , $\lambda=0.71073$ Å
Temperature	293(2) K
Scan type	θ -2 θ
Crystal system	Orthorhombic
Space group	Cmcm (No. 63)
Unit cell dimensions	$a = 4.6210(9)$ Å $b = 10.694(2)$ Å $c = 7.455(2)$ Å
Volume	$368.40(13)$ Å ³
Z	4
Density (calculated)	8.585 g/cm ³
Absorption coefficient	29.012 mm ⁻¹
F(000)	808
Crystal size	$0.19 \times 0.05 \times 0.04$ mm
θ range for data collection	3.81° to 27.48°
Index ranges	$-1 \leq h \leq 6$, $-1 \leq k \leq 13$, $-1 \leq l \leq 9$
Reflections collected	391
Independent reflections	255 ($R_{\text{int}} = 0.0305$)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.984 and 0.509
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	255/0/16
Goodness-of-fit on F^2	1.089
Final R indices ($I > 2\sigma(I)$)	$R_1 = 0.0310$, $wR_2 = 0.0614$
R indices (all data)	$R_1 = 0.0459$, $wR_2 = 0.0666$
Largest diff. peak and hole	2.547 and -1.546 eÅ ⁻³

TABLE 2

Atomic Coordinates^a and Equivalent Isotropic
Displacement Parameters ($\text{\AA}^2 \times 10^3$) for CePdIn₂

	x	y	z	U(eq)
In in 8(f)	0.0 [0.0]	0.3612(1) [0.1388]	0.0506(1) [0.0506]	11(1)
Ce in 4(c)	0.0 [0.0]	0.0756(1) [0.4244]	0.25 [0.25]	10(1)
Pd in 4(c)	0.0 [0.0]	0.7931(2) [0.7069]	0.25 [0.25]	11(1)

^aCoordinates in brackets are in STRUCTURE TIDY format.

TABLE 3

Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for CePdIn₂

	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃ =U ₁₂
Pd	9(1)	12(1)	10(1)	0	0
Ce	10(1)	11(1)	11(1)	0	0
In	11(1)	13(1)	8(1)	1(1)	0

TABLE 4

Interatomic Bond Distances (\AA)
for CePdIn₂

Ce	1Pd	3.021(3)
	2Pd	3.278(2)
	4In	3.2891(9)
	2In	3.396(2)
	4In	3.5786(13)
Pd	1Ce	3.021(3)
	2Ce	3.278(2)
	2In	2.783(2)
	4In	2.8421(9)
In	2Ce	3.2891(9)
	1Ce	3.396(2)
	2Ce	3.5786(13)
	1Pd	2.783(2)
	2Pd	2.8421(9)
	1In	2.973(2)
	1In	3.064(2)

LIST OF FIGURE CAPTIONS

FIG. 1. Structure of CePdIn_2 illustrating trigonal prismatic coordination around the Pd atoms.

FIG. 2. Local coordination environments around a) Ce b) Pd and c) In atoms. The dark lines indicate the pentagonal and trigonal prismatic units in the Ce and Pd coordination polyhedra.

FIG. 3. Inverse magnetic susceptibility as a function of temperature. Inset shows susceptibility vs temperature for $T < 50$ K.

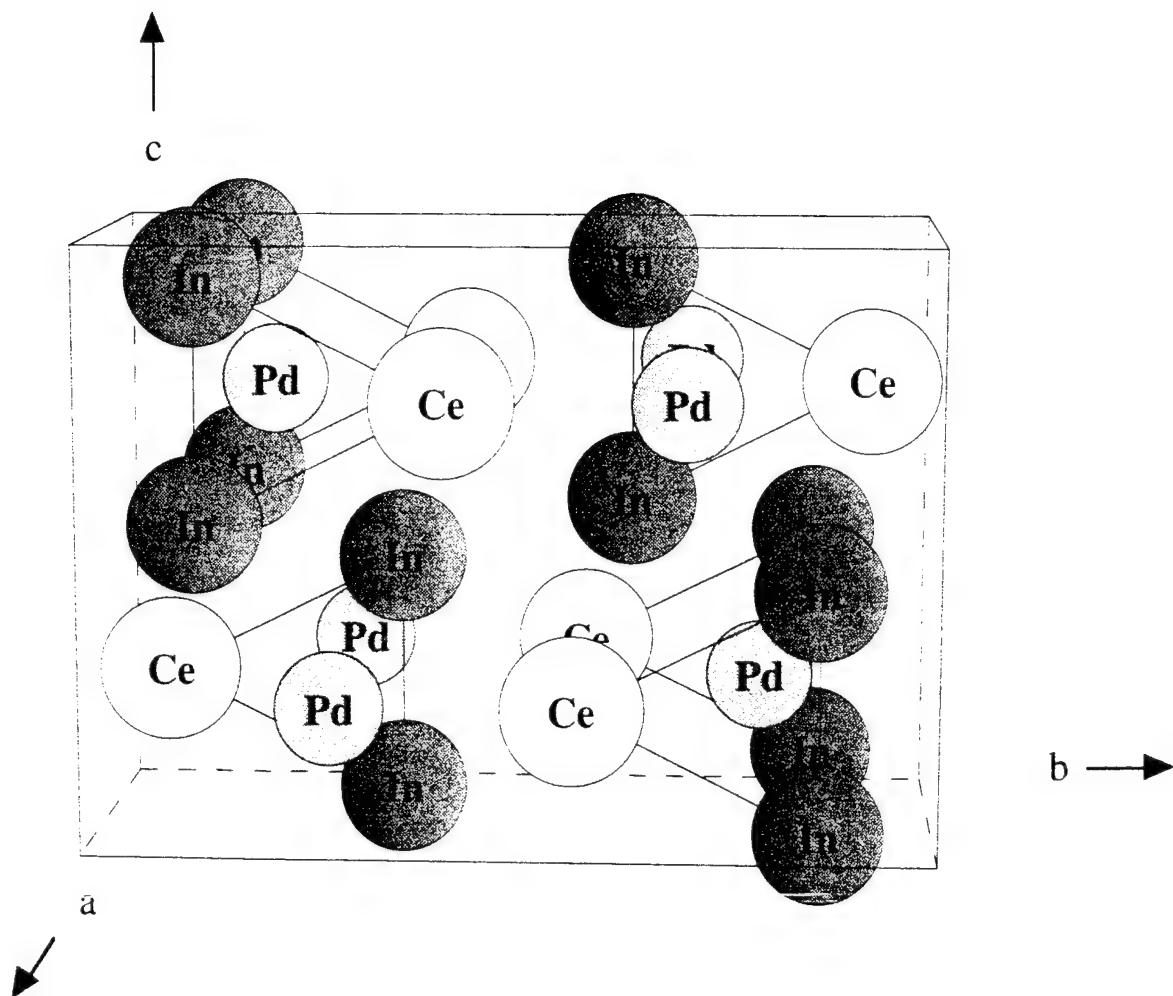
FIG. 4. Magnetic susceptibility vs inverse field at 4.2 K.

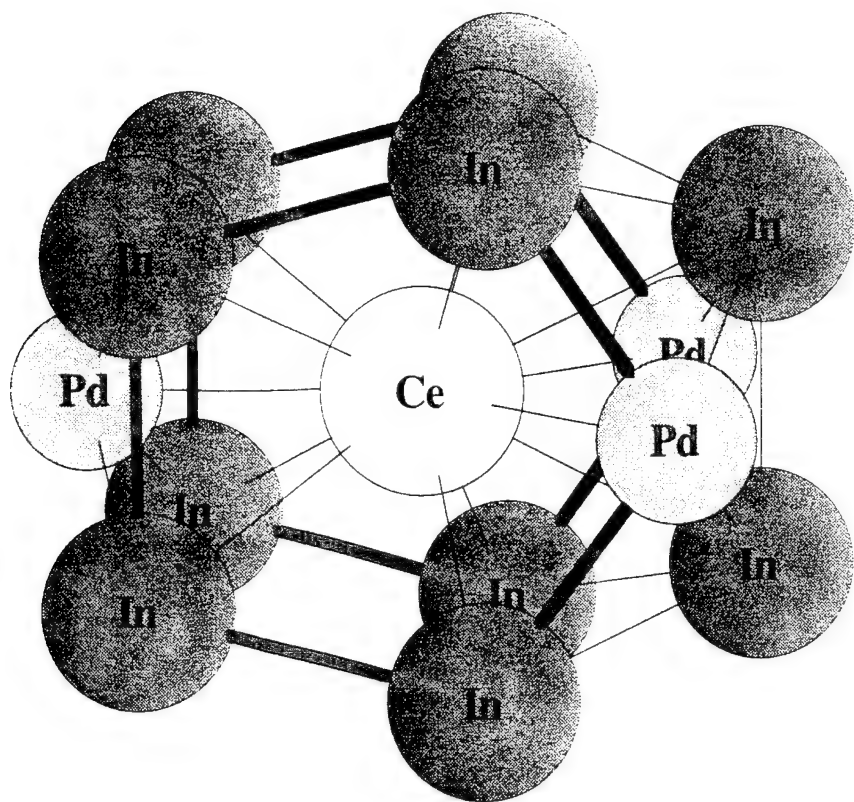
FIG. 5. Electrical resistivity as a function of temperature. Inset shows resistivity for $T < 25$ K.

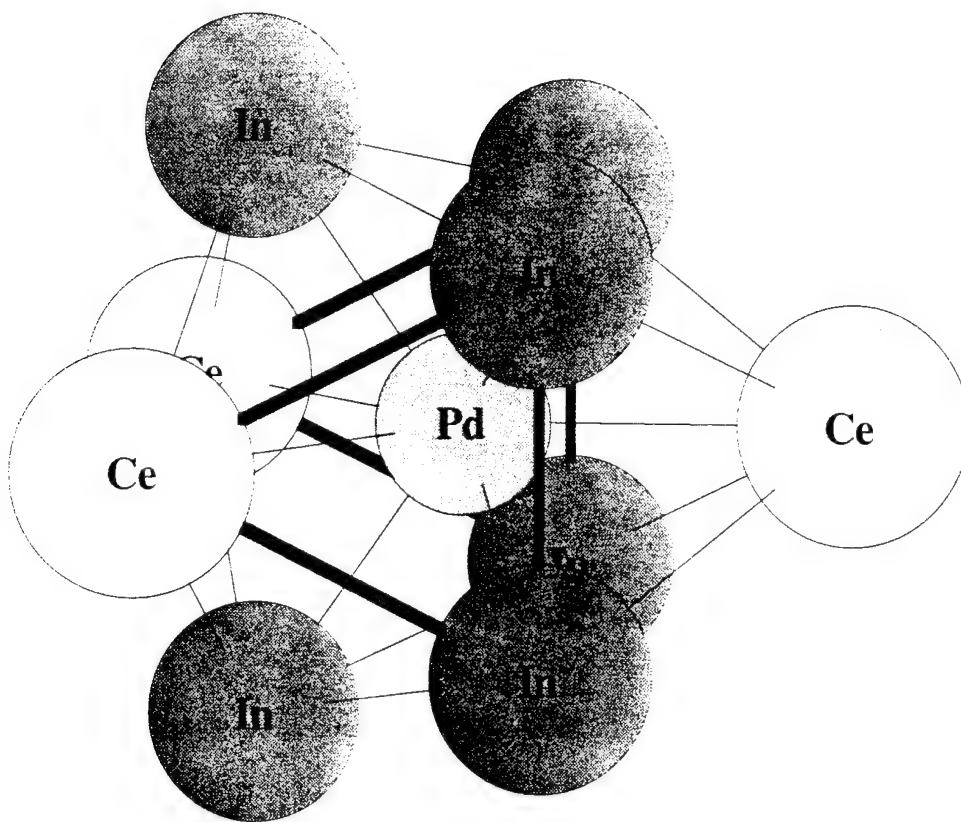
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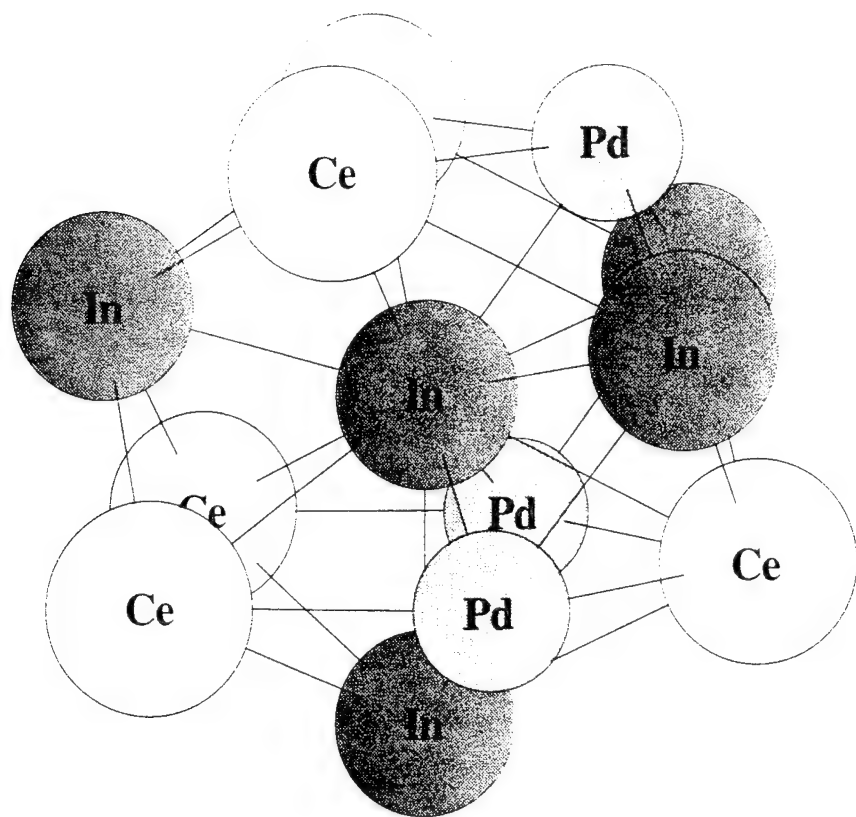
¹ See NAPS document No. __ for __ pages of supplementary material.

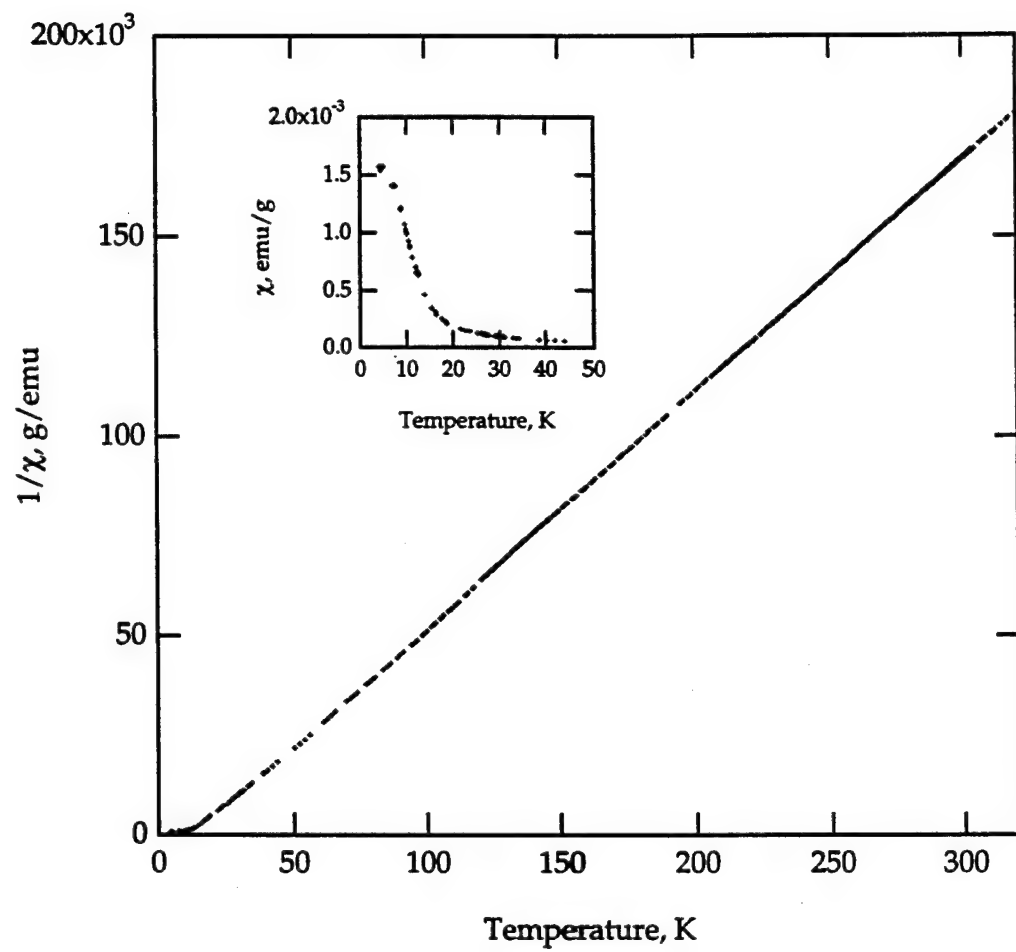
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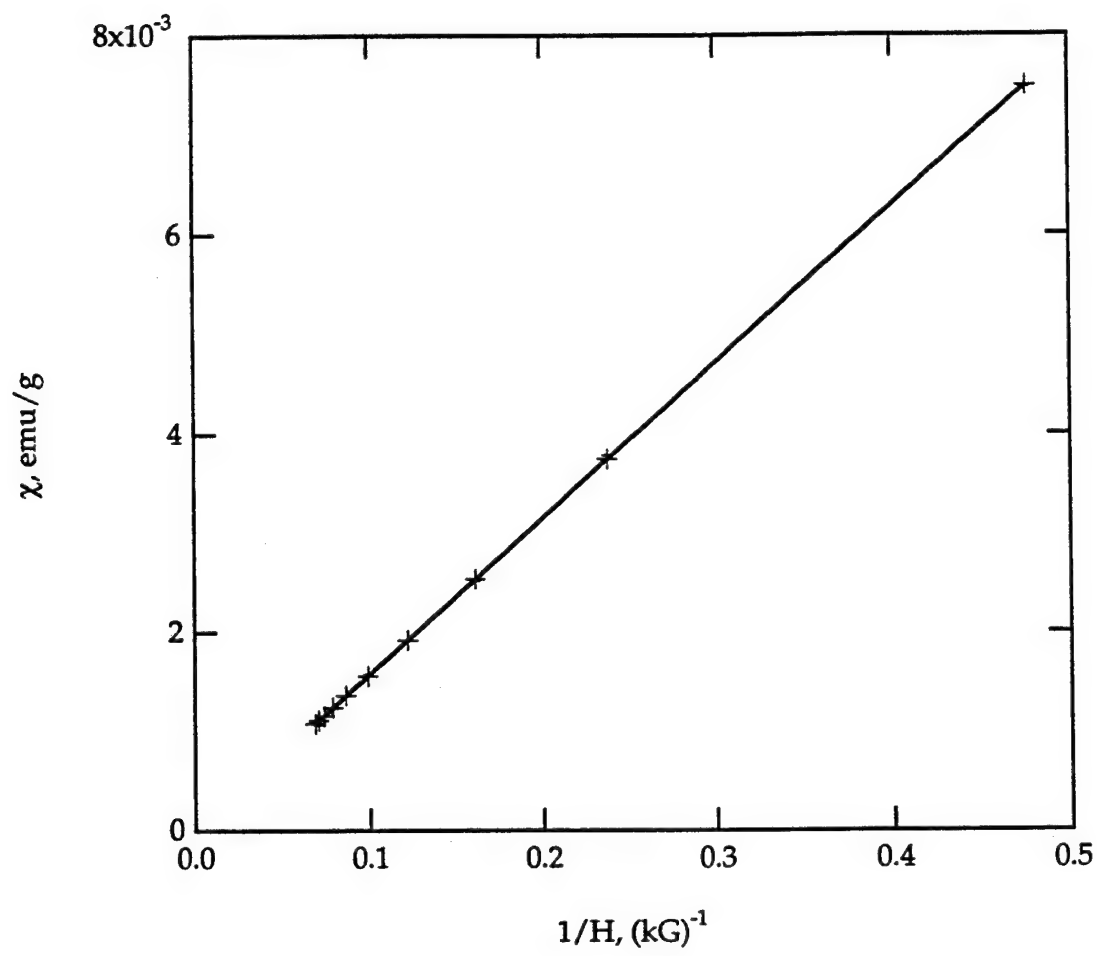


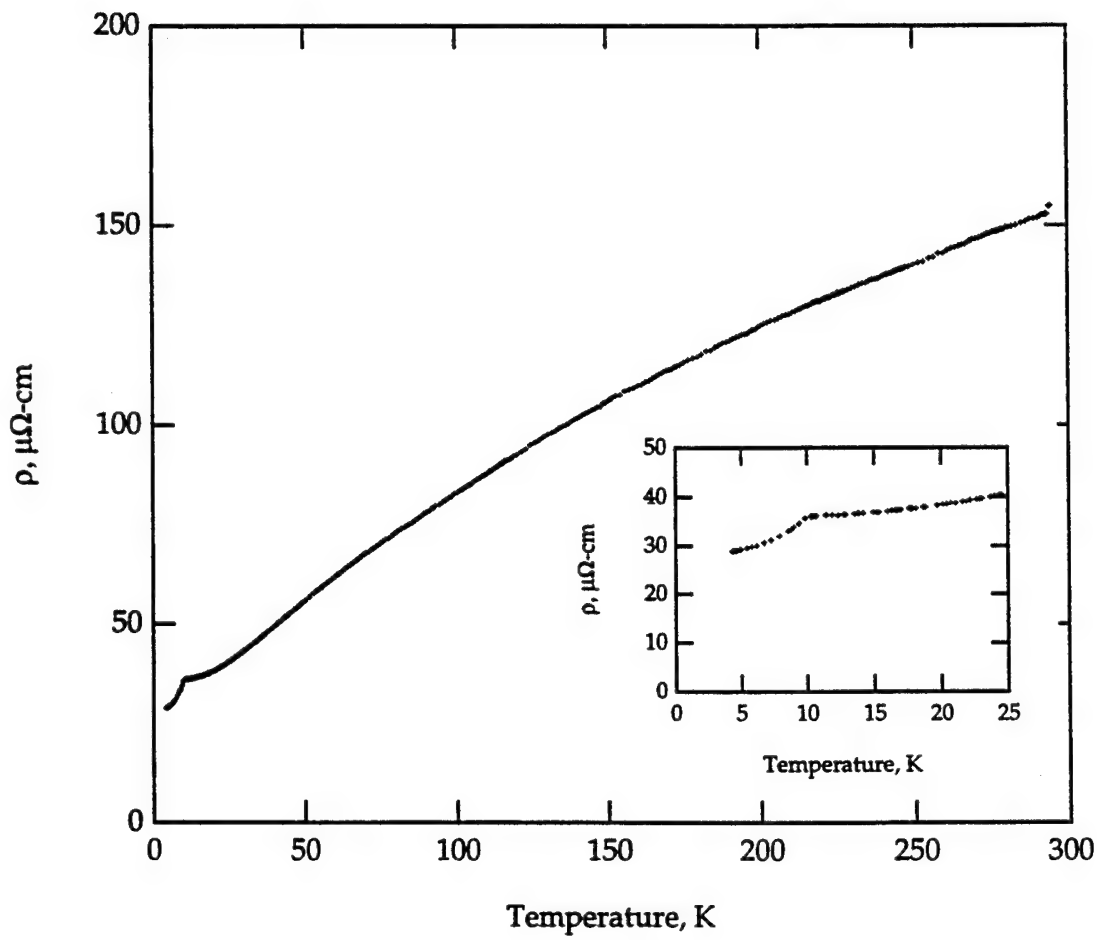












Supplementary information: observed and calculated structure factors

h k l 10Fo 10Fc 10s				h k l 10Fo 10Fc 10s				h k l 10Fo 10Fc 10s				h k l 10Fo 10Fc 10s				h k l 10Fo 10Fc 10s			
2	0	0	6254 6015 40	5	5	1	0 79 1	1	11	2	769 764 28	4	4	4	404 381 60	1	3	6	319 90 45
4	0	0	3912 3868 31	0	6	1	281 39 46	3	11	2	590 637 64	1	5	4	301 214 56	3	3	6	153 65 153
6	0	0	2435 2462 24	2	6	1	0 28 1	0	12	2	628 630 47	3	5	4	436 155 74	0	4	6	606 561 37
1	1	0	124 45 36	4	6	1	0 27 1	2	12	2	574 575 60	5	5	4	334 116 97	2	4	6	479 503 72
3	1	0	135 62 134	1	7	1	679 689 17	1	13	2	933 875 27	0	6	4	762 829 37	4	4	6	402 377 82
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5	7	0	2437 2453 25	1	1	2	3724 3660 43	1	7	3	201 217 116	4	2	5	1104 1025 27	1	5	7	1668 1651 25
0	8	0	0 45 1	3	1	2	2702 2604 29	3	7	3	0 183 1	3	3	5	2332 2390 33	3	5	7	1426 1385 38
2	8	0	217 26 167	5	1	2	1726 1707 23	0	8	3	953 956 32	0	4	5	2692 2741 38	0	6	7	1417 1421 30
4	8	0	0 38 1	0	2	2	201 265 80	2	8	3	873 846 39	2	4	5	2419 2443 42	2	6	7	1314 1303 39
1	9	0	176 51 176	2	2	2	286 242 49	4	8	3	683 638 47	4	4	5	1809 1847 26	1	7	7	194 177 193
3	9	0	151 40 150	4	2	2	0 186 1	1	9	3	1738 1714 26	1	5	5	1232 1182 60	0	8	7	663 677 50
0	10	0	628 532 41	1	3	2	2740 2738 29	3	9	3	1389 1411 33	3	5	5	921 929 38	2	8	7	675 627 64
2	10	0	438 470 63	3	3	2	1961 1966 37	0	10	3	503 469 55	0	6	5	1086 1104 30	1	9	7	1251 1219 36
4	10	0	238 341 238	5	3	2	1240 1281 26	2	10	3	345 438 107	2	6	5	936 982 42	0	0	8	248 322 105
1	11	0	1742 1784 22	0	4	2	2219 2216 46	1	11	3	1182 1211 57	4	6	5	740 726 48	2	0	8	229 308 200
3	11	0	1522 1490 30	2	4	2	1838 1848 46	3	11	3	1100 1039 38	1	7	5	742 726 26	1	1	8	1811 1802 12
0	12	0	589 551 46	4	4	2	1254 1246 30	0	12	3	1430 1386 29	3	7	5	611 604 56	3	1	8	1513 1524 22
2	12	0	551 507 56	1	5	2	685 649 20	2	12	3	1257 1278 36	0	8	5	1059 1036 32	0	2	8	289 171 81
1	13	0	276 184 136	3	5	2	558 514 40	1	13	3	1280 1250 84	2	8	5	955 937 42	2	2	8	0 153 1
1	1	1	236 187 14	5	5	2	275 343 116	0	0	4	3625 3578 36	1	9	5	1103 1105 23	1	3	8	1374 1391 20
3	1	1	221 164 46	0	6	2	2315 2295 46	2	0	4	3131 3068 36	3	9	5	890 929 49	3	3	8	1152 1181 47
5	1	1	90 105 89	2	6	2	1979 2005 45	4	0	4	2241 2202 26	0	10	5	2071 1982 27	0	4	8	1099 1156 30
0	2	1	232 251 42	4	6	2	1442 1465 30	1	1	4	1210 1166 25	2	10	5	1729 1825 35	2	4	8	1064 1061 45
2	2	1	228 175 35	1	7	2	544 521 33	3	1	4	952 921 17	1	11	5	1448 1428 24	1	5	8	417 405 48
4	2	1	127 70 127	3	7	2	472 460 52	5	1	4	653 656 33	0	0	6	2852 2806 33	0	6	8	1291 1278 31
1	3	1	3152 3265 20	5	7	2	296 366 120	0	2	4	191 262 96	2	0	6	2493 2513 41	2	6	8	1156 1180 48
3	3	1	2397 2345 25	0	8	2	2656 2685 41	2	2	4	240 209 109	4	0	6	1910 1915 24	1	7	8	395 257 56
5	3	1	1587 1566 17	2	8	2	2409 2395 37	4	2	4	94 136 94	1	1	6	889 858 12	1	1	9	64 85 64
0	4	1	3137 3244 32	4	8	2	1753 1808 28	1	3	4	0 38 1	3	1	6	712 718 24	0	2	9	0 35 1
2	4	1	2566 2699 28	1	9	2	0 47 1	3	3	4	0 28 1	0	2	6	337 175 65	2	2	9	355 34 124
4	4	1	1883 1878 21	3	9	2	197 39 197	5	3	4	191 9 190	2	2	6	268 151 151	1	3	9	1290 1318 21
1	5	1	174 71 50	0	10	2	1694 1693 38	0	4	4	590 602 36	4	2	6	139 117 139	0	4	9	1342 1359 30
3	5	1	201 84 78	2	10	2	1560 1536 34	2	4	4	572 528 49								

Supplementary information: additional bond lengths (Å) and angles (°)

In-Pd#1	2.783(2)	In-Pd#2	2.8421(9)
In-Pd#3	2.8421(9)	In-In#4	2.973(2)
In-In#5	3.064(2)	In-Ce#6	3.2891(9)
In-Ce#7	3.2891(9)	In-Ce#8	3.396(2)
In-Ce#2	3.5786(13)	In-Ce#3	3.5786(13)
Ce-Pd	3.021(3)	Ce-Pd#9	3.278(2)
Ce-Pd#10	3.278(2)	Ce-In#11	3.2891(9)
Ce-In#12	3.2891(9)	Ce-In#13	3.2891(9)
Ce-In#14	3.2891(9)	Ce-In#15	3.396(2)
Ce-In#8	3.396(2)	Ce-In#2	3.5786(13)
Ce-In#16	3.5786(13)	Ce-In#17	3.5786(13)
Pd-In#18	2.783(2)	Pd-In#4	2.783(2)
Pd-In#17	2.8421(9)	Pd-In#2	2.8421(9)
Pd-In#3	2.8421(9)	Pd-In#16	2.8421(9)
Pd-Ce#19	3.278(2)	Pd-Ce#20	3.278(2)
Pd#1-In-Pd#2	105.63(3)	Pd#1-In-Pd#3	105.63(3)
Pd#2-In-Pd#3	108.77(5)	Pd#1-In-In#4	143.65(4)
Pd#2-In-In#4	58.47(2)	Pd#3-In-In#4	58.47(2)
Pd#1-In-In#5	112.10(6)	Pd#2-In-In#5	112.15(5)
Pd#3-In-In#5	112.15(5)	In#4-In-In#5	104.26(4)
Pd#1-In-Ce#6	64.73(4)	Pd#2-In-Ce#6	168.55(4)
Pd#3-In-Ce#6	80.67(2)	In#4-In-Ce#6	132.95(2)
In#5-In-Ce#6	68.46(3)	Pd#1-In-Ce#7	64.73(4)
Pd#2-In-Ce#7	80.67(2)	Pd#3-In-Ce#7	168.55(4)
In#4-In-Ce#7	132.95(2)	In#5-In-Ce#7	68.46(3)
Ce#6-In-Ce#7	89.25(3)	Pd#1-In-Ce#8	79.60(4)
Pd#2-In-Ce#8	62.67(4)	Pd#3-In-Ce#8	62.67(4)
In#4-In-Ce#8	64.05(2)	In#5-In-Ce#8	168.30(6)
Ce#6-In-Ce#8	118.89(3)	Ce#7-In-Ce#8	118.89(3)
Pd#1-In-Ce#2	135.59(2)	Pd#2-In-Ce#2	54.69(5)
Pd#3-In-Ce#2	118.15(4)	In#4-In-Ce#2	65.46(2)
In#5-In-Ce#2	58.75(3)	Ce#6-In-Ce#2	127.21(3)
Ce#7-In-Ce#2	72.40(2)	Ce#8-In-Ce#2	113.23(3)
Pd#1-In-Ce#3	135.59(2)	Pd#2-In-Ce#3	118.15(4)
Pd#3-In-Ce#3	54.69(5)	In#4-In-Ce#3	65.46(2)
In#5-In-Ce#3	58.75(3)	Ce#6-In-Ce#3	72.40(2)
Ce#7-In-Ce#3	127.21(3)	Ce#8-In-Ce#3	113.23(3)
Ce#2-In-Ce#3	80.43(4)	Pd-Ce-Pd#9	135.19(3)
Pd-Ce-Pd#10	135.19(3)	Pd#9-Ce-Pd#10	89.62(6)
Pd-Ce-In#11	101.87(3)	Pd#9-Ce-In#11	50.14(2)
Pd#10-Ce-In#11	110.44(4)	Pd-Ce-In#12	101.87(3)
Pd#9-Ce-In#12	110.44(4)	Pd#10-Ce-In#12	50.14(2)
In#11-Ce-In#12	156.27(6)	Pd-Ce-In#13	101.87(3)
Pd#9-Ce-In#13	50.14(2)	Pd#10-Ce-In#13	110.44(4)
In#11-Ce-In#13	85.90(3)	In#12-Ce-In#13	89.25(3)
Pd-Ce-In#14	101.87(3)	Pd#9-Ce-In#14	110.44(4)
Pd#10-Ce-In#14	50.14(2)	In#11-Ce-In#14	89.25(3)
In#12-Ce-In#14	85.90(3)	In#13-Ce-In#14	156.27(6)
Pd-Ce-In#15	154.05(2)	Pd#9-Ce-In#15	50.36(3)
Pd#10-Ce-In#15	50.36(3)	In#11-Ce-In#15	61.11(3)
In#12-Ce-In#15	96.51(3)	In#13-Ce-In#15	96.51(3)
In#14-Ce-In#15	61.11(3)	Pd-Ce-In#8	154.05(2)
Pd#9-Ce-In#8	50.36(3)	Pd#10-Ce-In#8	50.36(3)
In#11-Ce-In#8	96.51(3)	In#12-Ce-In#8	61.11(3)

In#13-Ce-In#8	61.11(3)	In#14-Ce-In#8	96.51(3)
In#15-Ce-In#8	51.91(4)	Pd-Ce-In#2	50.15(2)
Pd#9-Ce-In#2	155.46(2)	Pd#10-Ce-In#2	89.98(3)
In#11-Ce-In#2	150.26(4)	In#12-Ce-In#2	52.79(3)
In#13-Ce-In#2	107.60(2)	In#14-Ce-In#2	87.78(2)
In#15-Ce-In#2	139.28(2)	In#8-Ce-In#2	113.23(3)
Pd-Ce-In#16	50.15(2)	Pd#9-Ce-In#16	155.46(2)
Pd#10-Ce-In#16	89.98(3)	In#11-Ce-In#16	107.60(2)
In#12-Ce-In#16	87.78(2)	In#13-Ce-In#16	150.26(4)
In#14-Ce-In#16	52.79(3)	In#15-Ce-In#16	113.23(3)
In#8-Ce-In#16	139.28(2)	In#2-Ce-In#16	49.08(4)
Pd-Ce-In#17	50.15(2)	Pd#9-Ce-In#17	89.98(3)
Pd#10-Ce-In#17	155.46(2)	In#11-Ce-In#17	52.79(3)
In#12-Ce-In#17	150.26(4)	In#13-Ce-In#17	87.78(2)
In#14-Ce-In#17	107.60(2)	In#15-Ce-In#17	113.23(3)
In#8-Ce-In#17	139.28(2)	In#2-Ce-In#17	100.30(5)
In#16-Ce-In#17	80.43(4)	In#18-Pd-In#4	107.29(7)
In#18-Pd-In#17	124.96(3)	In#4-Pd-In#17	74.37(3)
In#18-Pd-In#2	74.37(3)	In#4-Pd-In#2	124.96(3)
In#17-Pd-In#2	150.32(9)	In#18-Pd-In#3	74.37(3)
In#4-Pd-In#3	124.96(3)	In#17-Pd-In#3	63.07(4)
In#2-Pd-In#3	108.77(5)	In#18-Pd-In#16	124.96(3)
In#4-Pd-In#16	74.37(3)	In#17-Pd-In#16	108.77(5)
In#2-Pd-In#16	63.07(4)	In#3-Pd-In#16	150.32(9)
In#18-Pd-Ce	126.35(4)	In#4-Pd-Ce	126.35(4)
In#17-Pd-Ce	75.16(4)	In#2-Pd-Ce	75.16(4)
In#3-Pd-Ce	75.16(4)	In#16-Pd-Ce	75.16(4)
In#18-Pd-Ce#19	65.13(3)	In#4-Pd-Ce#19	65.13(3)
In#17-Pd-Ce#19	138.99(5)	In#2-Pd-Ce#19	66.97(3)
In#3-Pd-Ce#19	138.99(5)	In#16-Pd-Ce#19	66.97(3)
Ce-Pd-Ce#19	135.19(3)	In#18-Pd-Ce#20	65.13(3)
In#4-Pd-Ce#20	65.13(3)	In#17-Pd-Ce#20	66.97(3)
In#2-Pd-Ce#20	138.99(5)	In#3-Pd-Ce#20	66.97(3)
In#16-Pd-Ce#20	138.99(5)	Ce-Pd-Ce#20	135.19(3)
Ce#19-Pd-Ce#20	89.62(6)		

Symmetry transformations used to generate equivalent atoms:

- #1 $x, y, z+1$ #2 $-x-1/2, -y+1/2, -z+1$ #3 $-x+1/2, -y+1/2, -z+1$
#4 $x, y, -z+3/2$ #5 $-x, -y, -z+2$ #6 $x+1/2, y-1/2, z+1$
#7 $x-1/2, y-1/2, z+1$ #8 $-x, -y+1, -z+1$ #9 $x+1/2, y+1/2, z$
#10 $x-1/2, y+1/2, z$ #11 $x+1/2, y+1/2, -z+3/2$ #12 $x-1/2, y+1/2, z-1$
#13 $x+1/2, y+1/2, z-1$ #14 $x-1/2, y+1/2, -z+3/2$ #15 $-x, -y+1, z-1/2$
#16 $-x-1/2, -y+1/2, z-1/2$ #17 $-x+1/2, -y+1/2, z-1/2$ #18 $x, y, z-1$
#19 $x-1/2, y-1/2, z$ #20 $x+1/2, y-1/2, z$

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